

1,3-Dioxolane
646-06-0 | DTXSID4027284

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.55e-12 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.76e-01

Confidence level: 7.43e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Dioxane

Measured: 1.09e-11

Predicted: 7.30e-12

Image not found

2-Chloroethanol

Measured: 1.40e-12

Predicted: 2.40e-12

Image not found

Dimethoxymethane

Measured: 4.90e-12

Predicted: 6.85e-12

Image not found

1,3-Dioxane

Measured: 9.15e-12

Predicted: 1.03e-11

Image not found

2-Methyl-1,3-dioxolane

Measured: 9.40e-12

Predicted: 9.84e-12